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Disturbance spreading in incommensurate and quasiperiodic systems

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Abstract

The propagation of an initially localized excitation in 1D incommensurate, quasiperiodic and random systems is investigated numerically. It is discovered that the time evolution of variances $\sigma^2(t)$ of atom displacements depends on the initial condition. For the initial condition with nonzero momentum, $\sigma^2(t)$ goes as t^α with $\alpha = 1$ and 0 for incommensurate Frenkel-Kontorova (FK) model at V below and above V_c respectively; and $\alpha = 1$ for uniform, quasiperiodic and random chains. It is also found that $\alpha = 1 - \beta$ with β the exponent of distribution function of frequency at zero frequency, i.e., $\rho(\omega) \sim \omega^\beta$ (as $\omega \rightarrow 0$). For the initial condition with zero momentum, $\alpha = 0$ for all systems studied. The underlying physical meaning of this diffusive behavior is discussed.

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I. INTRODUCTION

The fast development of nanotechnology makes one-dimensional (1D) systems like quantum wire¹ and nanotubes² available in laboratories nowadays. The study of physical properties such as localization, thermal conductivity, and electron conductance, etc., in these systems become more and more important³. In the past years, many works have been done on the waves (classical and quantum) propagation and localization in 1D disordered media. Particular interests are paid to propagation of the classical waves in random media (see e.g.⁴), and electron transport in 1D disordered solids^{5,6}. In comparison with the disordered systems, much less is studied about the transport and diffusion properties of incommensurate and quasiperiodic systems, even though the incommensurate structures appear in many physical systems such as quasicrystals, two-dimensional electron systems, magnetic superlattices, charge-density waves, organic conductors, and various atomic monolayers absorbed on crystalline substrates⁷.

In this paper, we would like to study the classical transport of an initially localized excitation in 1D incommensurate, quasiperiodic and random systems so as to better understand transport processes and relaxations properties in these systems. Recently, quantum diffusion in two families of 1D models have attracted much attention^{8–10}. Typical examples are the kicked rotator and kicked Harper models from the field of quantum chaos, and the Harper model and the tight-binding model associated with quasiperiodic sequences. Many interesting dynamical behaviors, such as quantum localization and anomalous diffusion, and their relationships with energy spectra have been investigated in these systems^{8–10}. However, the classical transport in incommensurate and quasiperiodic systems and its relation with phonon frequency distribution, as well as the diffusive behavior dependence on initial condition, etc. have not yet fully investigated up to now.

The information of disturbance spreading in such system reflects the interior structures of the underlying system. As we shall see later, the spreading properties are determined largely by the density of states, in particular by the phonon model near the zero frequency.

II. MODELS AND NUMERICAL RESULTS

A. Incommensurate chain

The Frenkel-Kontorova (FK) model¹¹ is invoked as a prototype of an incommensurate chain in this paper. This model is a 1D atom chain with an elastic nearest neighbor interaction and subjected to an external periodic potential. Most works on this model in the past two decades have been concentrated on ground state properties and phonon spectra, etc. The 1D FK model is described by a dimensionless Hamiltonian

$$H = \sum_n \left[\frac{p_n^2}{2} + \frac{1}{2}(x_{n+1} - x_n - a)^2 - V \cos(x_n) \right], \quad (1)$$

where p_n and x_n are momentum and position of the n th atom, respectively. V is the coupling constant, and a is the distance between consecutive atoms without external potential. Aubry and Le Daëron¹² showed that the ground state configuration is commensurate when $a/2\pi$

is rational and incommensurate when $a/2\pi$ is irrational. For an incommensurate ground state, there are two different configurations separated by the so-called *transition by breaking of analyticity* predicted by Aubry¹³. This transition survives the quantum fluctuation¹⁴. Moreover, in contrast to other 1D nonintegrable systems such as the Fermi-Pasta-Ulam chain¹⁵, the FK chain shows a normal thermal conductivity¹⁶. For each irrational number $a/2\pi$ there exists a critical value V_c separating the sliding state ($V < V_c$) from pinned state ($V > V_c$). The $V_c = 0.9716354\cdots$ corresponds to the most irrational number, golden mean value $a/2\pi = (\sqrt{5} - 1)/2$. Without loss of generality, we restrict ourselves to this particular value of a in the numerical calculations throughout the paper, and it is approximated by a converging series of truncated fraction: F_n/F_{n+1} , where $\{F_n\}$ is the Fibonacci sequence.

The equation of motion for the n th atom in the FK model around its equilibrium position is

$$\frac{d^2\psi_n}{dt^2} = \psi_{n+1} + \psi_{n-1} - [2 + V \cos(x_n^0)]\psi_n, \quad (2)$$

where x_n^0 is the equilibrium position of the n th atom at ground state, and ψ_n is the normalized displacement from the equilibrium position. In fact, to obtain Eq.(2), we have written the whole displacement of particle as $x_n = x_n^0 + \epsilon\psi_n$, where $\epsilon(\ll 1)$ is a small parameter. To quantify the disturbance spreading, the variance of displacements

$$\sigma^2(t) = \frac{1}{N} \sum_{n=1}^N |\psi_n(t) - \psi_n(0)|^2 \quad (3)$$

is calculated by two numerical methods. The first one is the Runge-Kutta method of the fourth order to integrate Eq. (2) for a given initial condition with free boundary. The second one is to find eigenfrequencies ω_j and eigenvectors $\alpha_n(j)$ of equation

$$-\omega^2\psi_n = \psi_{n+1} + \psi_{n-1} - [2 + V \cos(x_n^0)]\psi_n. \quad (4)$$

The solution of Eq. (4) can be expressed in the following form:

$$\psi_n(t) = \sum_{j=1}^N [A_j \cos(\omega_j t) + B_j \sin(\omega_j t)] \alpha_n(j) \quad (5)$$

where the coefficients A_j and B_j are determined by initial conditions. Contrasting to the quantum diffusion, the classical evolution Eq. (2) is of the second order of derivative. Thus initial conditions for ψ_n and $d\psi_n/dt$ are needed. One of our main findings is that the spreading behavior depends on the initial condition. For the initial condition

$$\psi_n = 0 \text{ and } d\psi_n/dt = \delta_{n,n_0}$$

which is called type I, we have $\sigma^2 \sim t^\alpha$, and α is equal to 1 and 0 for $V < V_c$ and $V > V_c$, respectively. For the initial condition

$$\psi_n = \delta_{n,n_0} \text{ and } d\psi_n/dt = 0$$

which is called type II, $\sigma^2 \sim t^0$ for any V . (Of course, there is another type of initial condition, i.e., $\psi_n = \delta_{n,n_0}$ and $d\psi_n/dt = \delta_{n,n_0}$. Our numerical calculations show that the

spreading behavior in this case is the same as that of type-I initial condition.) Figure 1 shows the typical time evolution $\sigma^2(t)$ for the FK model. In numerical calculations, we first obtain the ground state positions of N atoms in the FK chain by the gradient method for free boundary, i.e., $x_0 \equiv 0$ and $x_N = Na$. The results of Fig. 1 are obtained by the integration method for $N = F_{19} = 10946$. $\sigma^2(t)$ is also calculated by the second numerical method for the FK chains of small size, which gives rise to the same results.

It is worth pointing out that the above-mentioned results valid only for the evolution time less than a critical value t^* , where $t^* \sim N/2v$ and v is the velocity of sound. For our FK model, $v \approx 1$. After this critical time, i.e., $t > t^*$, the power relation of $\sigma^2(t) \sim t^\alpha$ is destroyed due to the finite size effect.

To get a clear picture of the spreading of a disturbance in an incommensurate chain with two different initial conditions, we plot $\psi_n(t)$ in Fig. 2 for the FK chain of $V = 0.4$. The intensity of gray scale represents the amplitude of the displacement of the particle. Because of the huge amount of the data, we record $\psi_n(t)$ at a time interval of 20 time steps, which leads to some discontinuity. Figure 2(a) demonstrates the evolution with initial condition $\psi_n = 0$ and $d\psi_n/dt = \delta_{n,n_0}$, and Fig. 2(b) shows that with initial condition $\psi_n = \delta_{n,n_0}$ and $d\psi_n/dt = 0$. The difference is clear. In the later case the disturbance spreads out in both direction, and the particle remains almost at rest after the disturbance passes it. However, in the first case, wherever the disturbance spreads, the particle will be excited and keeps moving. In the cantorus regime ($V > V_c$), the disturbance spreading in the FK chain is similar to the case in Fig. 2(b) regardless of the initial condition.

B. Quasiperiodic and random chains

We turn now to study of disturbance spreading in uniform, quasiperiodic, and random chains. The equation of motion can be written as

$$\frac{d^2\psi_n(t)}{dt^2} = k_n\psi_{n+1} + k_{n-1}\psi_{n-1} - (k_n + k_{n-1})\psi_n. \quad (6)$$

If $k_n = k$ for all n , it corresponds to a uniform chain. For quasiperiodic chains, k_n takes two values k_1 and k_2 which are arranged according to some deterministic quasiperiodic substitute rules¹⁷. Here we discuss four types of quasiperiodic chains. They are Fibonacci, Thue-Morse, Rudin-Shapiro, and period-doubling chains, respectively. The substitute rules for them are: $k_1 \rightarrow k_1k_2, k_2 \rightarrow k_1$ (Fibonacci); $k_1 \rightarrow k_1k_2, k_2 \rightarrow k_2k_1$ (Thue-Morse); $k_1k_1 \rightarrow k_1k_1k_1k_2, k_1k_2 \rightarrow k_1k_1k_2k_1, k_2k_1 \rightarrow k_2k_2k_1k_2, k_2k_2 \rightarrow k_2k_2k_2k_1$ (Rudin-Shapiro); $k_1 \rightarrow k_1k_2, k_2 \rightarrow k_1k_1$ (period-doubling). According to the classification based on the eigenvalues of generating matrix defined by Luck¹⁸, they are bounded (Fibonacci, Thue-Morse), unbounded (Rudin-Shapiro), and marginal (period-doubling). For comparison, $\sigma^2(t)$ for random chain is also studied. In this case, the values of k_n are taken k_1 and k_2 with the same probability. Figure 3 shows typical time evolutions of variances for four quasiperiodic and random chains. The disturbance spreading behaviors in these chains are the same as that of the incommensurate FK model at $V < V_c$, namely, $\sigma^2(t) \sim t$ for all these chains with the initial condition of nonzero momentum [$d\psi_n(0)/dt \neq 0$], and t^0 for all these chains with initial condition of zero momentum [$d\psi_n(0)/dt = 0$].

C. Relationship with phonon spectrum

Figures 1-3 are the main results. They demonstrate that the disturbance spreading depends crucially on the initial condition. In the following, we would like to understand this peculiar behavior in terms of the phonon spectra.

The coefficients A_j and B_j in Eq. (5) are: $A_j = 0$ and $B_j = \alpha_{n_0}(j)/\omega_j$ for type-I boundary condition; $A_j = \alpha_{n_0}(j)$ and $B_j = 0$ for type II. Therefore the solutions of Eq. (2) are

$$\begin{aligned}\psi_n &= \sum_{j=1}^N \sin(\omega_j t) \alpha_n(j) \alpha_{n_0}(j) / \omega_j, & \text{type I,} \\ \psi_n &= \sum_{j=1}^N \cos(\omega_j t) \alpha_n(j) \alpha_{n_0}(j), & \text{type II,}\end{aligned}\quad (7)$$

respectively. As $N \rightarrow \infty$, we have

$$\begin{aligned}\frac{1}{N} \sum_{n=1}^N \psi_n^2 &\sim \int_{\omega_{min}}^{\omega_{max}} \sin^2(\omega t) \alpha_{n_0}^2 \rho(\omega) d\omega / \omega^2, & \text{type I,} \\ \frac{1}{N} \sum_{n=1}^N \psi_n^2 &\sim \int_{\omega_{min}}^{\omega_{max}} \cos^2(\omega t) \alpha_{n_0}^2 \rho(\omega) d\omega & \text{type II,}\end{aligned}\quad (8)$$

respectively, where $\omega_{max}/\omega_{min}$ is the maximum/minimal frequency of phonon spectra and $\rho(\omega)$ is the density of the phonon spectra.

The difference between the integrands in Eq. (8) for type I and type II lies in the factor $1/\omega^2$. As time increases, the dominant contribution of the integral in Eq. (8) for type I comes from the integrand around $\omega = 0$. The integrand for type II is an oscillated function of time t , and so is the integral. Therefore the reason for different behaviors of these chains for different initial conditions is due to the coefficients B_j in Eq. (5). If B_j is equal to zero, i.e., the initial condition with zero momentum, $\sigma^2(t)$ is an oscillated function of time. If B_j is nonzero, i.e., the initial condition with nonzero momentum, $\sigma^2(t)$ is proportional to t .

In fact, the integral in Eq. (8) for type-I boundary condition can be written as

$$\int_{\omega_{min} t}^{\omega_{max} t} t \sin^2(\tilde{\omega}) \alpha_{n_0}^2 \rho(\frac{\tilde{\omega}}{t}) d\tilde{\omega} / \tilde{\omega}^2. \quad (9)$$

If the distribution function of frequency has the scaling behavior $\rho(\omega) \sim \omega^\beta$ at low frequency ($\omega \rightarrow 0$), then one has $\alpha = 1 - \beta$. For the uniform chain, it is well known that $\rho(\omega) = 2/(\pi \sqrt{\omega_m^2 - \omega^2})$, thus $\beta = 0$. We also discover that for the Fibonacci chain and random chain, the distribution function of frequency at low frequency are the same as that of uniform chain^{6,19}. To demonstrate this, we calculate the integrated distribution function of frequency (IDFF) for these quasiperiodic chains by directly diagonalizing chains of finite length, and plot them in Fig. 4 as a function of ω . The results suggest that for all these quasiperiodic chains the IDFF is proportional to ω at low frequency, thus $\beta = 0$, which is the same as that of uniform and random chains so that the relationship $\alpha = 1 - \beta$ is satisfied for all these systems.

For the incommensurate FK model, it is well known that there is a zero-frequency phonon mode for $V < V_c$, whereas there is a phonon gap for $V > V_c$. From above discussion, we know that the zero-frequency phonon mode plays a key role in the time behavior of $\sigma^2(t)$. The time behavior of $\sigma^2(t)$ in the incommensurate FK chain at $V < V_c$ suggests that the low frequency behavior of distribution function of frequency is the same as that of those chains discussed above. The curves shown in Fig. 4 indeed demonstrate this. But for the incommensurate FK chain at $V > V_c$, $\omega_{min} > 0$, thus the integral in Eq. (8) for type I is an oscillated function and the time behavior of $\sigma^2(t)$ is also an oscillated function of time. The case $V = V_c$ is critical. The phonon spectrum of the FK chain at V_c is different from that of $V < V_c$. It has self-similar structure and is point spectrum [see Fig. 5(a)]. Therefore there is no inverse power relation between $\rho(\omega)$ and ω at low frequency. It implies that the results would depend on the length of the chain in numerical calculation. This is illustrated in Fig. 5(b), where we plot $\sigma^2(t)$ as a function of t for the FK chains of different length at $V = V_c$.

III. CONCLUSION AND DISCUSSIONS

We have studied the disturbance spreading in incommensurate, uniform, quasiperiodic and random chains. We have found that the time evolution of variance $\sigma^2(t)$ depends on the initial conditions. Its behavior is determined by the density of phonon frequency around zero frequency. For the initial condition of zero momentum, $\sigma^2(t) \sim t^0$ for all kinds of chains studied in this letter. For the initial condition of nonzero momentum, $\sigma^2(t) \sim t^\alpha$, $\alpha = 1$ for uniform, quasiperiodic, random chains, and incommensurate FK chain at $V < V_c$. Although other physical properties differs from system to system, the time behavior of $\sigma^2(t)$ are the same for all these systems. For the incommensurate FK chain at $V > V_c$, $\sigma^2(t)$ is an oscillated function of time. This different behavior of the incommensurate FK chain at different V regimes might provide us a different approach to detect the transition by breaking of analyticity experimentally.

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FIGURES

FIG. 1. $\sigma^2(t)$ of the incommensurate FK chains with different values of V for different initial conditions. The solid and dotted lines correspond to $V = 0.4$ and $V = 1.6$, respectively. (a) Initial condition $\psi_n(0) = 0$ and $d\psi_n(0)/dt = \delta_{n,n_0}$; (b) initial condition $\psi = \delta_{n,n_0}$ and $d\psi_n(0)/dt = 0$. The length of the FK chain is $N = 10946$. Initial excitation locates at the center of the chain, namely, $n_0 = N/2 + 1$.

FIG. 2. Time evolution of the displacement $\psi_n(t)$ for an incommensurate FK chain of $V = 0.4$ with different initial conditions: (a) $\psi_n(0) = 0$ and $d\psi_n(0)/dt = \delta_{n,n_0}$; (b) $\psi = \delta_{n,n_0}$ and $d\psi_n(0)/dt = 0$. The length of the FK chain is $N = 1597$. The initial excitation locates at the middle of the chain, i.e., $n_0 = 799$.

FIG. 3. $\sigma^2(t)$ of quasiperiodic and random chains with different initial conditions. The solid, dotted, dashed, long dashed, and dot-dashed lines correspond to Fibonacci, Thue-Morse, period-doubling, Rudin-Shapiro, and random chains, respectively. (a) Initial condition $\psi_n(0) = 0$ and $d\psi_n(0)/dt = \delta_{n,n_0}$; (b) initial condition $\psi = \delta_{n,n_0}$ and $d\psi_n(0)/dt = 0$. The chain length is $N = 10946$ for the Fibonacci chain and $N = 8192$ for the Thue-Morse, period-doubling, Rudin-Shapiro, and random chains.

FIG. 4. The integrated distribution function of frequency (IDFF) as a function of ω at low frequency for different chains. The solid, dotted, dashed, long dashed, and dot-dashed lines correspond to the Fibonacci, Thue-Morse, period-doubling, Rudin-Shapiro chains, and the incommensurate FK chain at $V < V_c$, respectively. The results are obtained by directly diagonalizing chains of finite length. The chain length is $N = 1597$ for the Fibonacci and the FK chain, and $N = 2048$ for the Thue-Morse, period-doubling, and Rudin-Shapiro chains.

FIG. 5. (a) The distribution function of frequency D as a function of ω at low frequency for the incommensurate FK at $V = V_c$. (b) the time evolution of variance $\sigma^2(t)$ in the incommensurate FK chain at $V = V_c$ for different lengths. The initial condition is $\psi_n(0) = 0$ and $d\psi_n(0)/dt = \delta_{n,n_0}$.

Fig. 1 (Hu et al.)

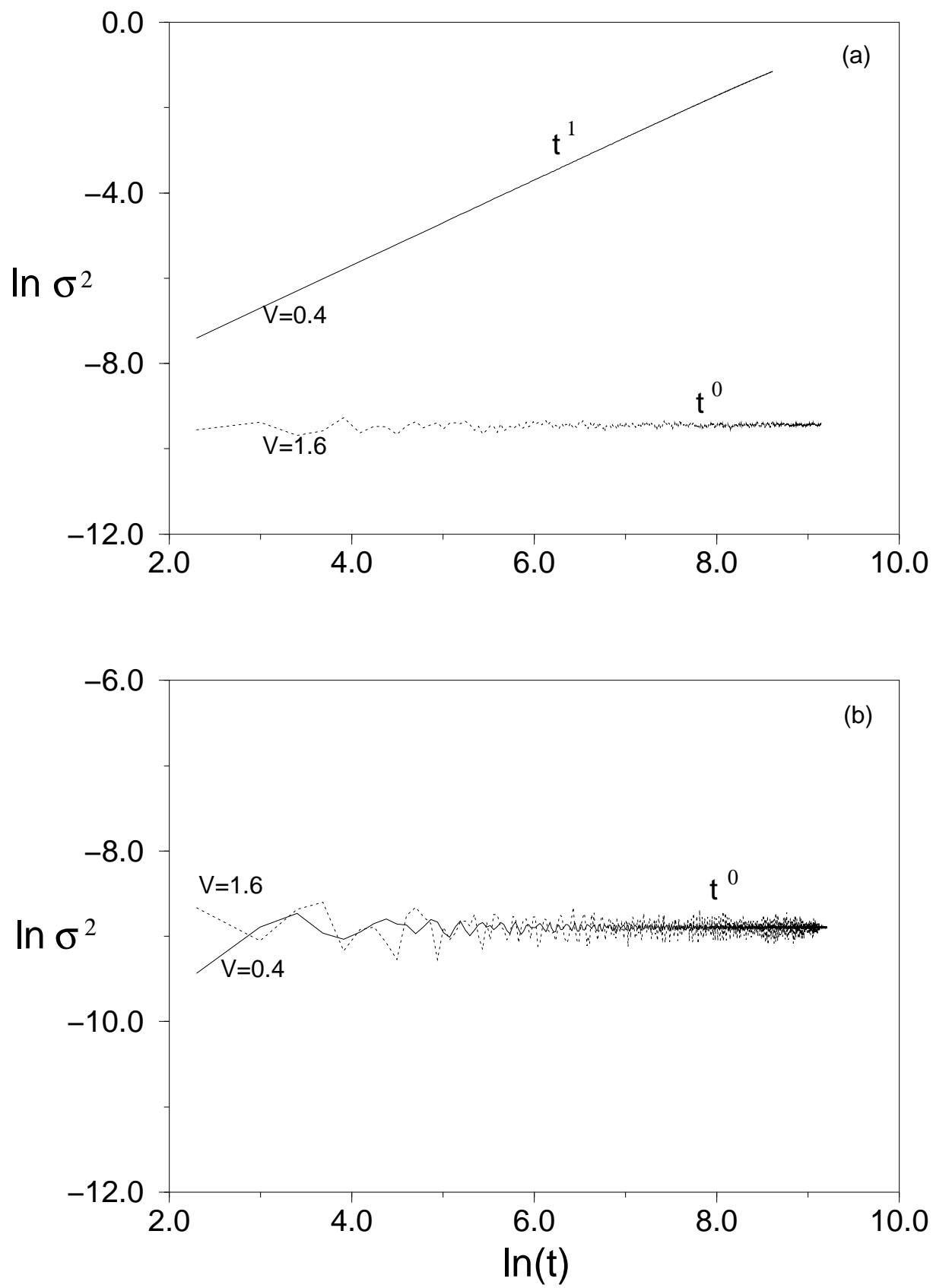


Fig. 2 (Hu et al.)

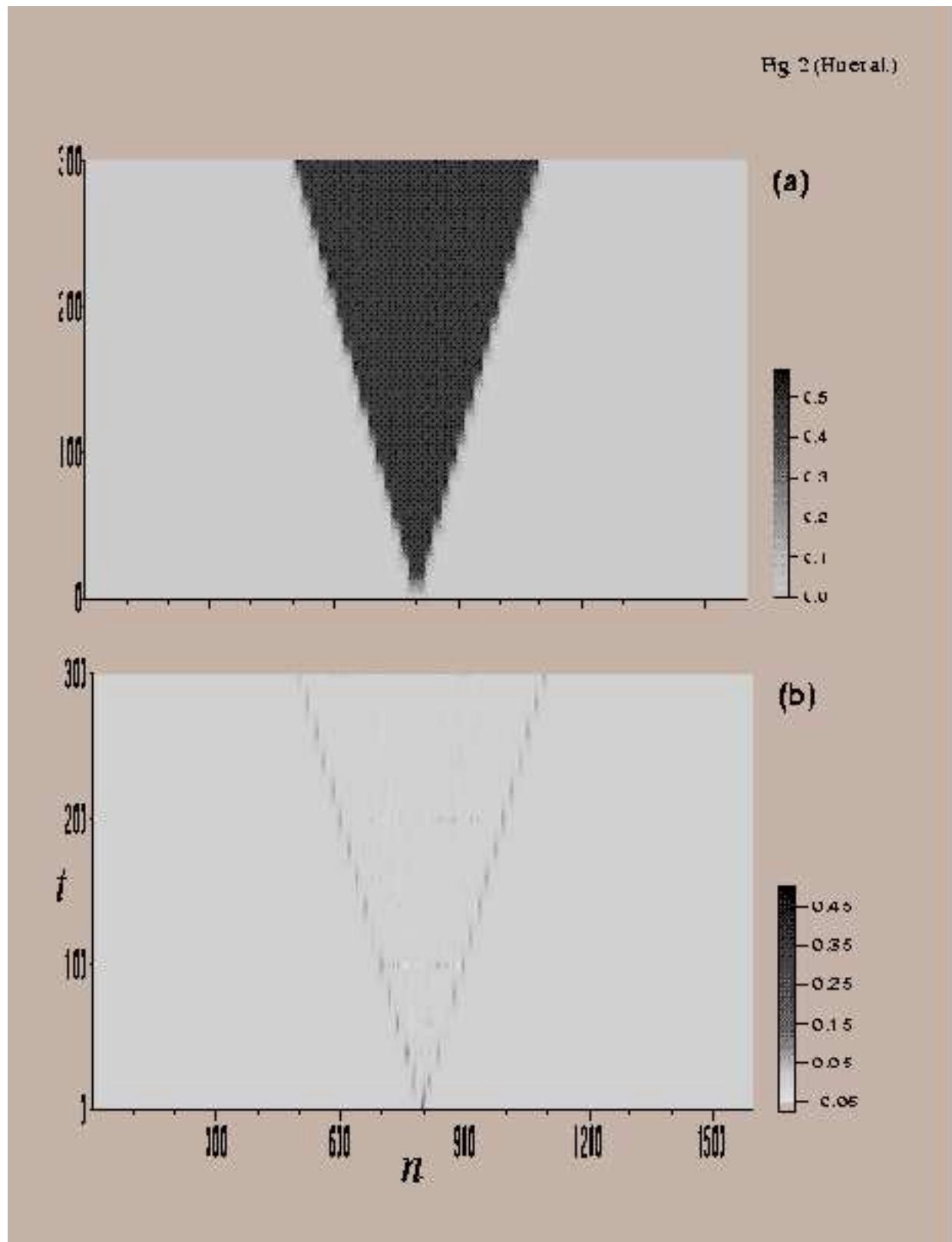


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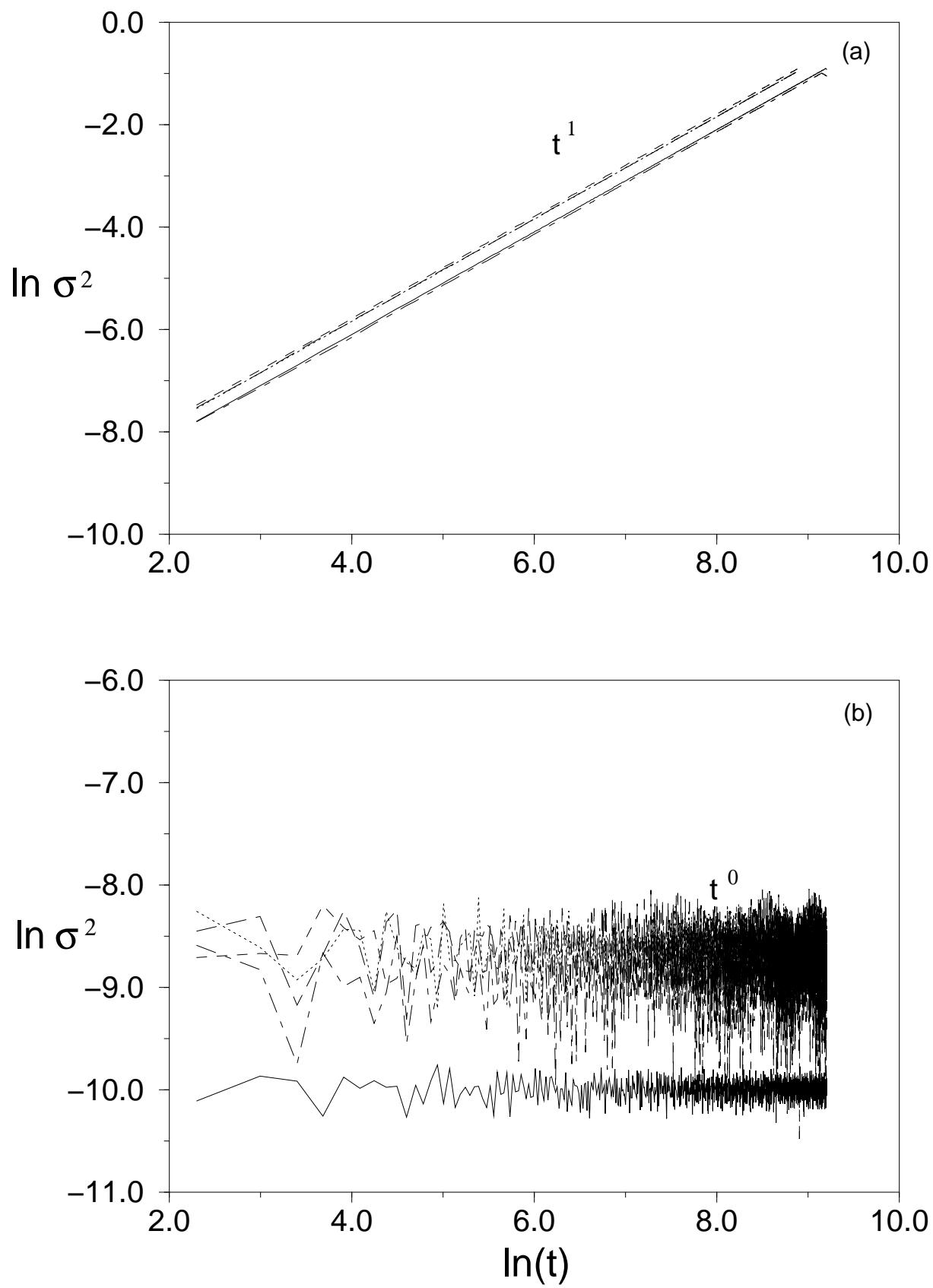


Fig. 4 (Hu et al.)

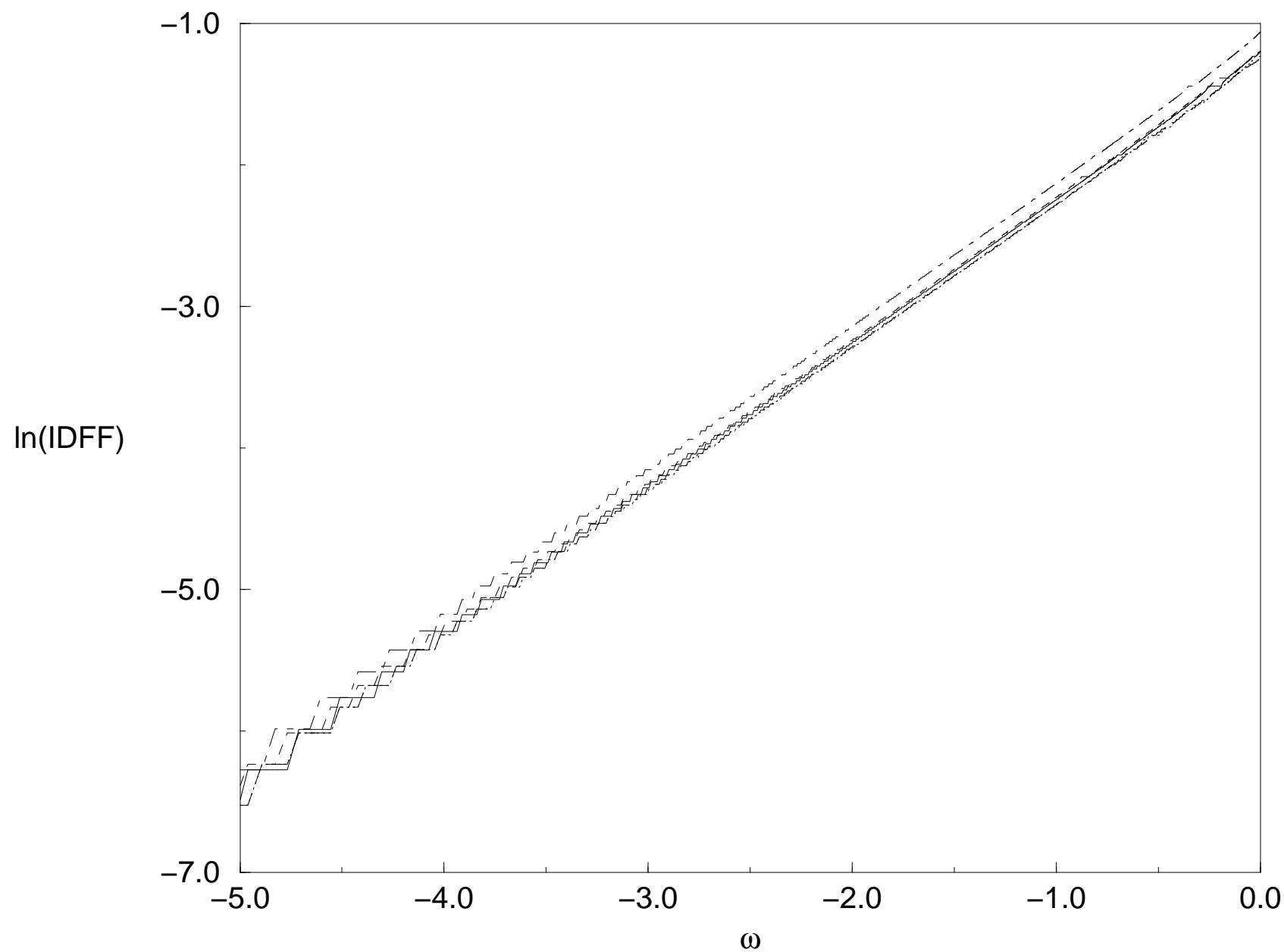


Fig. 5 (Hu et al.)

